NAME SOLUTIONS

FIRST EXAM

MSE102

Thursday September 30th 2010

One side of an 8.5x11" sheet and a calculator is allowed. Closed book and notes.

1. SHORT ANSWER QUESTIONS
   a. Why do atoms form bonds? What are the relevant interactions among atoms that result in the formation of bonds. Give an example of a material and the type(s) of bond found in it. [6]

Since a completely filled shell is the most stable electronic configuration for an atom, atoms tend to form bonds such that the shells of both atoms become completely filled. The bonding is described as a balance between coulomb attraction at long distances due to bond formation lowering energy and short range repulsion associated with Pauli's exclusion principle.

ex: graphite (C) composed of covalently bonded C atom sheets that interact via van der Waal's between sheets.

   b. What is the relationship between a real space lattice and the corresponding reciprocal lattice? [4]

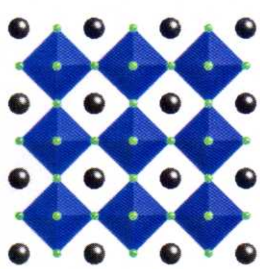
Reciprocal lattice points represent planes in real space. The reciprocal lattice vectors indicate the direction of the surface normal of the plane in real space and the magnitude of the reciprocal lattice vector represents the inverse of the wavelength of the parallel set of real space planes:

$$|\vec{G}_{hkl}| = \frac{1}{\lambda_{hkl}}$$

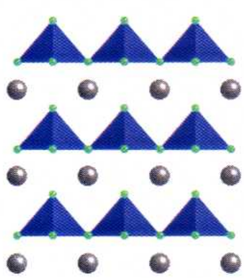
c. Are the reciprocal lattices of a simple cubic lattice (lattice constant ***a*** on a side) with a basis of one atom and a simple cubic lattice (lattice constant ***a*** on a side) with a basis of two atoms, the same or different? Explain. [4]

The reciprocal lattices are identical as they represent the planes in real space associated with the real space lattice and lattice points. The choice of basis has no bearing on the lattice.

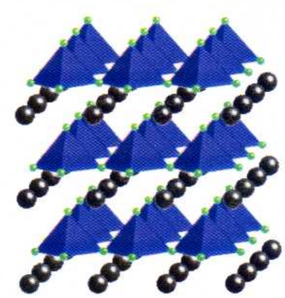
d. For the crystal structure shown to the right, vanadium ions are the electropositive ions and oxygen are the electronegative ions of the square pyramidal polyhedra which are interleaved with the Pb ions shown as balls. What is the stoichiometry of this material? Explain. [6]



(001) view



(100) view



In a unit cell

there are 8 Pb atoms shared by 8 other unit cells → 1 Pb

there is one V atom shared by no other unit cell → 1 V

there are 4 O atoms shared by two other unit cells → 2 O

there is one O atom shared by one other unit cell → 1 O

$\Rightarrow PbVO_3$

e. Consider a set of planes of the form $(h\bar{h}l)$. What is the zone axis of this set of planes? [4]

The zone axis must obey the zone equation:

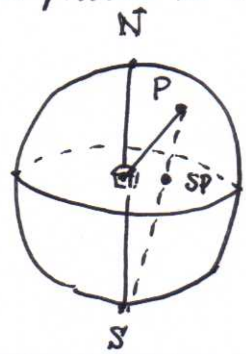
$hu - hv + lw = 0$ where $\underline{t}$ = zone axis vector = $u\underline{a} + v\underline{b} + w\underline{c}$ (translation vectors)

for the set of planes $(h\bar{h}l)$. Not only is the plane normal $\hat{n} \cdot \vec{t} = 0$ but also $\hat{n}_1 \times \hat{n}_2$ must point in the $\vec{t}$ direction for $\hat{n}_1$ and $\hat{n}_2$ being two plane normals corresponding to $(h_1 \bar{h}_1 l_1)$ and $(h_2 \bar{h}_2 l_2)$.

Calculating $\hat{n}_1 \times \hat{n}_2 = [u\ u\ 0]$. So [110] would be an example.

f. How does one determine the stereographic projection of a single crystal sample? Explain with a diagram. [6]

For a point P on a sphere that denotes a plane normal or simply a direction relative to a single crystal placed at the origin of the sphere, project a line from a pole in the opposite hemisphere. The intersection of this projection line with the equatorial plane is the stereographic projection point.

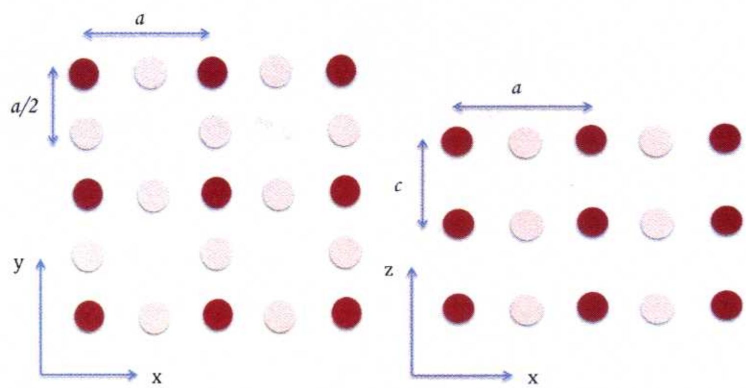


Problem #1.______/30

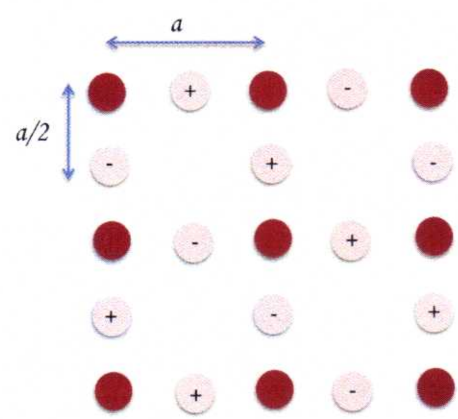
Problem#2._____/30

Total:_____/60

2. Consider 3D lattice below composed of two types of atoms (dark and light). Layers of this two dimensional pattern on the left are stacked on top of one another a distance *c* apart as shown on the right.

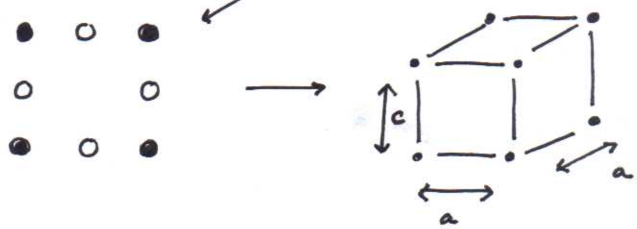


(a) Sketch the Bravais lattice.[2]
(b) What are the primitive translation vectors? [6]
(c) Sketch the unit cell. [4]
(d) What is the basis? [3]
(e) Write down a general expression for a reciprocal lattice vector for this structure. [3]
(f) Sketch and label lengths on the reciprocal lattice. [4]
(g) If some of the light atoms are actually displaced above the plane of the dark atoms and other light atoms are displaced below as indicated by the + and - signs by a distance $\delta \ll a/2$, what is the primitive cell and lattice for this new lattice? [3]



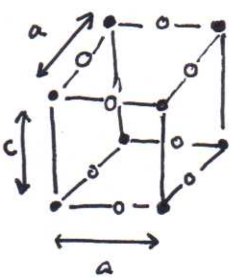
(h) What is the corresponding reciprocal lattice? [3]
(i) What can we say about how distortions in the crystal lattice affect the reciprocal lattice? [2]

(a) Bravais lattice of the following structure stacked on top of one another a distance c apart is tetragonal



(b) primitive translation vectors are $\underline{a}_1 = a\hat{x}$, $\underline{a}_2 = a\hat{y}$, $\underline{a}_3 = c\hat{z}$

(c) the unit cell is a simple cubic unit cell — $a \times a \times c$



(d) The basis is made up of 3 atoms

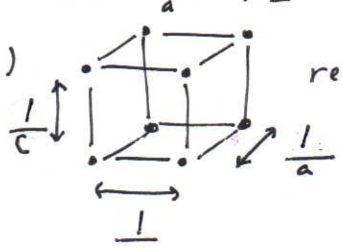
one dark : (0, 0, 0)
one white : $(\frac{1}{2}, 0, 0)$
one white : $(0, \frac{1}{2}, 0)$

(i) The distortions effectively decreases the spacing between reciprocal lattice points in the xy plane while keeping the spacing along the z-axis the same. In addition, the orientation of the unit cell is rotated by 90° due to the distortion and this rotation is also reflected in the reciprocal lattice.

(e) the general expression for a reciprocal lattice vector: $\vec{G}_{hkl} = h\underline{a}_1^* + k\underline{a}_2^* + l\underline{a}_3^*$ where $\underline{a}_1^*$, $\underline{a}_2^*$: $\underline{a}_3^*$ are the reciprocal lattice vector for the tetragonal lattice are:

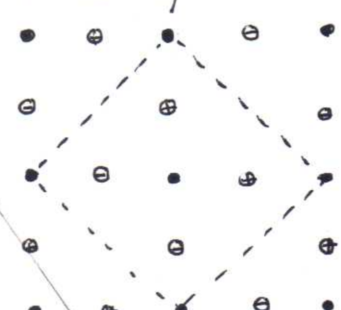
$$\underline{a}_1^* = \frac{1}{a}\hat{x}\ ,\ \underline{a}_2^* = \frac{1}{a}\hat{y}\ .\ \underline{a}_3^* = \frac{1}{c}\hat{z}$$

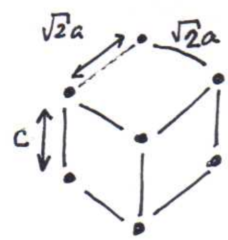
(f)



reciprocal lattice

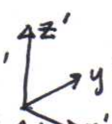
(g) If some of the atoms are displaced, the new Bravais lattice is





ORTHORHOMBIC.

(h) The corresponding reciprocal lattice can be derived from the orthorhombic primitive translation vectors



$$\underline{a}_1' = \sqrt{2}a\hat{x}\ ,\ \underline{a}_2' = \sqrt{2}a\hat{y}'\ .\ \underline{a}_3' = c\hat{z}'$$

are: $\underline{a}_1^* = \frac{1}{\sqrt{2}a}\hat{x}'$; $\underline{a}_2^{*\prime} = \frac{1}{\sqrt{2}a}\hat{y}'$; $\underline{a}_3^* = \frac{1}{c}\hat{z}'$

So the reciprocal lattice is an orthorhombic unit cell